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THE CRYSTAL STRUCTURE OF Cr_3B_4

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The Crystal Structure of Cr_3B_4

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A number of borides isostructural with Ta_3B_4 have already been investigated by Andersson and Kiessling^{1,2,3}. From his data on Mn_3B_4 Kiessling⁴ concluded that there are boron-boron distances as short as 1.50 Å in this phase and he believed these short boron-boron distances to be present also in the other Me_3B_4 phases³. The value 1.5 Å is considerably shorter than any boron-boron distance previously reported. However, the atomic parameters are very uncertain. A reinvestigation of these compounds is therefore being undertaken in order to achieve greater accuracy. The present communication deals with the results obtained for the alloy Cr_3B_4 .

Experimental: The alloys were prepared by arc-melting mixtures of boron (99.0 %) and chromium (99.9 %) in an atmosphere of purified argon. X-ray photographs were taken in a Guinier camera with Si as internal standard ($a_{\text{Si}} = 5.4306$ Å) and with $\text{CrK}\alpha$ -radiation. The atomic parameters were determined from single crystal data, obtained in a Weissenberg camera with $\text{MoK}\alpha$ -radiation. The relative intensities were estimated visually using the multiple film technique and a calibrated intensity scale. The electron density projection $\rho(xy)$, the structure factors and the scale- and temperature factors were computed and refined on the digital electronic

computer BESK with programs available at BESK. The scattering factors according to Watson and Freeman ⁵ for chromium and Ibers ⁶ for boron were used.

Results: Within the limits of the experimental errors (estimated to be $\pm 0.04\%$) no lattice parameter variations were observed. The lattice parameters of Cr_3B_4 obtained in this investigation ($a = 2.986 \text{ \AA}$, $b = 13.020 \text{ \AA}$, $c = 2.952 \text{ \AA}$) are in excellent agreement with Anderson's and Kiessling's ¹ values ($a = 2.984 \text{ \AA}$, $b = 13.02 \text{ \AA}$, $c = 2.953 \text{ \AA}$).

The space group Immm derived by Kiessling in his study of Ta_3B_4 was confirmed. The atomic parameters obtained in this investigation for Cr_3B_4 are given in Table 1. with standard deviations calculated from Cruickshank's formula ⁷. The final R-value for the 94 independent h_k0 reflexions was 7.6 %.

Interatomic distances are given in Table 2. Of particular interest are the shortest boron-boron distances, which have a standard deviation of 0.02 \AA . The difference between the two shortest non-equivalent boron-boron distances is not significant. Thus it has been shown that in Cr_3B_4 there exists no such abnormally short boron-boron distances as suggested by Kiessling ³.

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4. Kiessling, R. ibid. 4 (1950) 146.
5. Watson, R.E. and Freeman, A.J. Acta Cryst. 14 (1961) 27.
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Table 1. Atomic parameters in Cr_3B_4

Cr_I in 2(c)

Cr_II in 4(g) with $y = 0.1861 \pm 0.0000_6$

B_I in 4(g) with $y = 0.3607 \pm 0.0003$

B_II in 4(h) with $y = 0.4351 \pm 0.0003$

Table 2. Interatomic distances in Cr_3B_4 shorter than 3 Å

$\text{Cr}_\text{I} - \text{Cr}_\text{I}$	2.952 (2), 2.986 (2)
$\text{Cr}_\text{I} - \text{Cr}_\text{II}$	2.83 ₇ (4)
$\text{Cr}_\text{I} - \text{B}_\text{I}$	2.35 (4)
$\text{Cr}_\text{I} - \text{B}_\text{II}$	2.26 (8)
$\text{Cr}_\text{II} - \text{Cr}_\text{I}$	2.83 ₇ (2)
$\text{Cr}_\text{II} - \text{Cr}_\text{II}$	2.67 ₉ (4), 2.952 (2), 2.986 (2)
$\text{Cr}_\text{II} - \text{B}_\text{I}$	2.19 (4), 2.27 (1)
$\text{Cr}_\text{II} - \text{B}_\text{II}$	2.17 (2)
$\text{B}_\text{I} - \text{Cr}_\text{I}$	2.35 (2)
$\text{B}_\text{I} - \text{Cr}_\text{II}$	2.19 (4), 2.27 (1)
$\text{B}_\text{I} - \text{B}_\text{I}$	2.952 (2), 2.986 (2)
$\text{B}_\text{I} - \text{B}_\text{II}$	1.77 (2)
$\text{B}_\text{II} - \text{Cr}_\text{I}$	2.26 (4)
$\text{B}_\text{II} - \text{Cr}_\text{II}$	2.17 (2)
$\text{B}_\text{II} - \text{B}_\text{I}$	1.77 (2)
$\text{B}_\text{II} - \text{B}_\text{II}$	1.69 (1), 2.952 (2), 2.986 (2)